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Density Of Electron States In Wurtzite-Like Boron Nitride: A Quasi-Classical Calculation



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ABSTRACT

Using the parameterization based on the quasi-classical atomic orbitals the density of electron states for boron nitride in the wurtzite structure is obtained. The upper valence, gap, and lower conduction bandwidths of w-BN are estimated as 13.6eV, 5.4eV, and 11.6eV, respectively.

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KEYWORDS

Density of states;
Quasi-classical
approximation;
Wurtzite-like boron nitride.

INTRODUCTION

Boron nitride can be found in form of one-dimensional diatomic molecule BN; two-dimensional fullerene and nanotubular surfaces with the same chemical formula; three-dimensional layered hexagonal h-BN (with two-layer stacking sequence) and rhombohedral r-BN (with three-layer stacking sequence), densely packed cubic zinc-blende c-BN and wurtzite-like w-BN crystals. Besides, the multi-walled tubes and multi-shelled cage molecules on the base of BN, turbostratic and amorphous boron nitride films may be prepared. Boron nitrides are the materials with a diversity of industrial applications.

Among them the wurtzite-like modification also is of special scientific and technological interest being known for their superior bonding properties^[1] that are especially valuable in high-temperature applications. The hardness, high melting point, high thermal conductivity, large bulk modulus, etc make w-BN useful for protective coatings. It is chemically inert and does not react with iron. As a result the super-hard materials made from w-BN found applications in metal cutting operations. Furthermore, the electronic properties of w-BN characterized by large band gap and relatively low dielectric constant indicate^[2] its device applications in short-wavelength (green, blue, and ultraviolet) electro-luminescent

optics and high-temperature microelectronics.

As the substances can be considered as an electron systems affected by the stationary field of nuclei fixed at the sites in a structure of atoms, their physical and chemical properties are mainly determined by electron spectra, and for this reason it is important to calculate them. Applying the theoretical method based on the quasi-classical approximation the electron energy spectra were obtained for BN diatomic molecule^[3], isolated BN-layer^[4], hexagonal^[5], and cubic^[6] boron nitride crystals. In the present work in same way we calculate the density-of-states (DOS) of wurtzite phase. The paper is organized as follows. At first the used theoretical method is reviewed. Then results of the quasi-classical calculations are given. Finally they are discussed in comparison with experimental and theoretical data available for the w-BN electronic structure.

THEORETICAL BASIS

Success of quasi-classical approach to substance is explained by the diffuseness of atomic potentials. The expression for bounded electron states energies obtained by Maslov^[6] yields that precise and quasi-classical spectra are close to one another independently from the potential smoothness properties if the characteristic values of potential Φ_0 and the radius of its action R_0 meet requirement $\Phi_0 R_0^2 \gg 1$ (all relations are given in atomic units (au)). For atomic potential $\Phi_0 \sim Z/R$ and $R_0 \sim R$ where Z is the atomic number, $Z \geq 1$, and R is the radius of electron cloud. Therefore, in case of atoms it must be $2ZR \gg 1$. Even for light atoms R is several times larger than Bohr radius, $R \gg 1$. Thus, atoms and polyatomic structures – molecules and crystals – are quasi-classical electron systems in the sense specified. On this basis the quasi-classical approach to calculation of crystalline electronic structures has been developed (summarization see in^[7]). Its essential content can be described as follows.

The values of i th electron classical turning points radii r'_i and r''_i inside the constituent atom ($r'_i < r''_i$) are obtained by solving the equations

$$E_i = -\Phi_i(r) + I_i(I_i+1)/2r^2 \quad i = 1, 2, 3, \dots, Z,$$

Where r denotes the distance from the center of atom, $\Phi_i(r)$ is the potential affecting the given electron, $E_i < 0$ and I_i are its energy and orbital quantum number. At the ground state the inner classical turning point for relative motion of atomic nucleus and electron cloud coincides with the center of system. The outer classical turning point radius \tilde{r} is obtained by solving the equation $\tilde{E} = Z\tilde{\Phi}(r)$, where $\tilde{E} < 0$ denotes the energy associated with relative motion, and $\tilde{\Phi}(r) = -\left(Z^2/r - \sum_{i=1}^{i=Z} \Phi_i(r)\right)/(Z-1)$ is the electron cloud potential affecting the nucleus. In particular, using the quasi-classical parameterization based on the Coulomb-like atomic potentials $\Phi_i(r) = Z_i/r$ we get exact formulas

$$r'_i = n_i \left(n_i - \sqrt{n_i^2 - I_i(I_i+1)} \right) / Z_i,$$

$$r''_i = n_i \left(n_i + \sqrt{n_i^2 - I_i(I_i+1)} \right) / Z_i,$$

$$\tilde{r} = 2(Z-1) / Z^2 \left(Z^2 - \sum_{i=1}^{i=Z} Z_i \right)^2$$

$$\tilde{E} = -Z^3 \left(Z^2 - \sum_{i=1}^{i=Z} Z_i \right)^2 / 2(Z-1)^2$$

Here $Z_i = n_i \sqrt{2|E_i|}$ is the effective charge of the screened nucleus for i th electron and n_i is its principal quantum number.

The quasi-classical limit means the truncation of electron states charge densities outside the classical turning points and space averaging within the range between them. In this case i th electron partial charge density is approximated by the piecewise-constant radial function

$$\rho_i(r) = \begin{cases} 0 & r < r'_i \\ = -3/4\pi(r_i^{*3} - r_i'^3) & r'_i \leq r \leq r_i'' \\ = 0 & r_i'' < r, \end{cases}$$

Whereas the nucleus charge density is averaged inside the \tilde{r} -sphere:

$$\tilde{\rho}(r) = \begin{cases} 3Z/4\pi\tilde{r}^3 & 0 \leq r \leq \tilde{r} \\ = 0 & \tilde{r} < r \end{cases}$$

Consequently, full atomic charge density is expressed by the step-like radial function

$$\rho(r) = \tilde{\rho}(r) + \sum_{i=1}^{i=Z} \rho_{(i)}(r) = \rho_k$$

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$$r_{k-1} \leq r < r_k \quad k=1,2,3,\dots,q,$$

where r_k and ρ_k denote known constants that depend on parameters r'_i, r''_i and \tilde{r} , $0 \equiv r_0 < r_1 < r_2 < \dots < r_q < r_{q+1} \equiv \infty$, $q \leq 2Z$ is the number of 'homogenous' charge density radial layers in atom. Using the Poisson equation the radial dependence of the full atomic potential also can be approximated by the step-like function if substituted by the space-averaged values inside $r_{k-1} \leq r < r_k$ intervals:

$$\varphi(r) \approx \frac{3a_k(r_k^2 - r_{k-1}^2)}{2(r_k^3 - r_{k-1}^3)} + \frac{3b_k(r_k^5 - r_{k-1}^5)}{5(r_k^3 - r_{k-1}^3)} + c_k = \varphi_k$$

$$r_{k-1} \leq r < r_k \quad k=1,2,3,\dots,q$$

$$a_k = \sum_{i=1}^{i=k-1} 4\pi\rho_i(r_i^3 - r_{i-1}^3) / 3 - 4\pi\rho_k r_{k-1}^3 / 3$$

$$b_k = -2\pi\rho_k / 3$$

$$c_k = \sum_{i=k+1}^{i=q} 2\pi\rho_i(r_i^2 - r_{i-1}^2) + 2\pi\rho_k r_k^2$$

In the region $r > r_q$ the both of charge density and potential vanish identically ($\rho(r) \equiv 0$ and $\varphi(r) \equiv 0$). Thus, finite parameter r_q is the quasi-classical atomic radius.

Approximating the crystalline inner potential by the superposition of quasi-classical step-like potentials of constituent atoms and choosing the square roots of their piecewise-constant partial electron densities as basis set of wave functions the electronic spectrum $E = E(\vec{p})$ (\vec{p} denotes the electron quasi-momentum) is determined by solving the secular equation $\det(H - ES) = 0$ in which matrix elements of overlapping integrals S and Hamiltonian H are calculated

$$H_{(i)j(k)l}(\vec{p}) - ES_{(i)j(k)l}(\vec{p}) \rightarrow \begin{pmatrix} \text{Re } H_{(i)j(k)l}(\vec{p}) - E \text{Re } S_{(i)j(k)l}(\vec{p}) & \text{Im } H_{(i)j(k)l}(\vec{p}) - E \text{Im } S_{(i)j(k)l}(\vec{p}) \\ -\text{Im } H_{(i)j(k)l}(\vec{p}) + E \text{Im } S_{(i)j(k)l}(\vec{p}) & \text{Re } H_{(i)j(k)l}(\vec{p}) - E \text{Re } S_{(i)j(k)l}(\vec{p}) \end{pmatrix}$$

using the $r'_i, r''_i, \tilde{r}, r_k$ and φ_k parameters for constituent atoms ($r_{(i)j}$ is the radius of j th 'homogenous' potential radial layer in the (i) th atom; $\varphi_{(i)j}$ is the potential value inside this layer; $r_{(kz)\vec{r}-\vec{r}}$ is the displacement between (k) th and (K) th atoms of the unit cells, which are displaced from the central one by the translational vectors \vec{r} and \vec{r} , respectively):

$$S_{(i)j(k)l}(\vec{p}) = -\frac{3}{4\pi} \sum_{\vec{r}} \frac{V_{(ik)j\vec{r}}(r_{(ik)\vec{r}})}{\sqrt{(r_{(i)j}^{\#3} - r_{(i)j}^{\prime\prime 3})(r_{(k)l}^{\#3} - r_{(k)l}^{\prime\prime 3})}} \exp(i\vec{p}\vec{r})$$

$$V_{(ik)j\vec{r}}(r_{(ik)\vec{r}}) = V(r_{(i)j}, r_{(k)l}, r_{(ik)\vec{r}}) + V(r_{(i)j-1}, r_{(k)l-1}, r_{(ik)\vec{r}}) -$$

$$-V(r_{(i)j}, r_{(k)l-1}, r_{(ik)\vec{r}}) - V(r_{(i)j-1}, r_{(k)l}, r_{(ik)\vec{r}}),$$

$$H_{(i)j(k)l}(\vec{p}) = -\frac{3}{4\pi} \sum_{\vec{r}} \sum_{\vec{r}} \sum_{(\kappa)=1}^{(\kappa)=N} \sum_{\lambda=1}^{\lambda=q(\kappa)}$$

$$\frac{\varphi_{(\kappa)\lambda} V_{(ik\kappa)j\vec{r}}(r_{(ik)\vec{r}}, r_{(i\kappa)\vec{r}}, r_{(k\kappa)\vec{r}-\vec{r}})}{\sqrt{(r_{(i)j}^{\#3} - r_{(i)j}^{\prime\prime 3})(r_{(k)l}^{\#3} - r_{(k)l}^{\prime\prime 3})}} \exp(i\vec{p}\vec{r})$$

$$V_{(ik\kappa)j\vec{r}}(r_{(ik)\vec{r}}, r_{(i\kappa)\vec{r}}, r_{(k\kappa)\vec{r}-\vec{r}}) =$$

$$\begin{aligned} &= V(r_{(i)j}, r_{(k)l}, r_{(\kappa)\lambda}, r_{(ik)\vec{r}}, r_{(i\kappa)\vec{r}}, r_{(k\kappa)\vec{r}-\vec{r}}) + \\ &+ V(r_{(i)j}, r_{(k)l-1}, r_{(\kappa)\lambda-1}, r_{(ik)\vec{r}}, r_{(i\kappa)\vec{r}}, r_{(k\kappa)\vec{r}-\vec{r}}) + \\ &+ V(r_{(i)j-1}, r_{(k)l}, r_{(\kappa)\lambda-1}, r_{(ik)\vec{r}}, r_{(i\kappa)\vec{r}}, r_{(k\kappa)\vec{r}-\vec{r}}) + \\ &+ V(r_{(i)j-1}, r_{(k)l-1}, r_{(\kappa)\lambda}, r_{(ik)\vec{r}}, r_{(i\kappa)\vec{r}}, r_{(k\kappa)\vec{r}-\vec{r}}) - \\ &- V(r_{(i)j-1}, r_{(k)l}, r_{(\kappa)\lambda}, r_{(ik)\vec{r}}, r_{(i\kappa)\vec{r}}, r_{(k\kappa)\vec{r}-\vec{r}}) - \\ &- V(r_{(i)j}, r_{(k)l-1}, r_{(\kappa)\lambda}, r_{(ik)\vec{r}}, r_{(i\kappa)\vec{r}}, r_{(k\kappa)\vec{r}-\vec{r}}) - \\ &- V(r_{(i)j}, r_{(k)l}, r_{(\kappa)\lambda-1}, r_{(ik)\vec{r}}, r_{(i\kappa)\vec{r}}, r_{(k\kappa)\vec{r}-\vec{r}}) - \\ &- V(r_{(i)j-1}, r_{(k)l-1}, r_{(\kappa)\lambda-1}, r_{(ik)\vec{r}}, r_{(i\kappa)\vec{r}}, r_{(k\kappa)\vec{r}-\vec{r}}) \end{aligned}$$

They are the linear combinations of two universal geometric functions. The first $V = V(R_1, R_2, D_{12})$ expresses the dependence of two spheres' intersection region volume upon their radii R_1 and R_2 and inter-central distance D_{12} . It is a continuous piecewise analytical combination of algebraic functions. Another universal geometric function $V = V(R_1, R_2, R_3, D_{12}, D_{13}, D_{23})$ expressing the dependence of three spheres' intersection region volume upon their radii R_1, R_2, R_3 and inter-central distances D_{12}, D_{13}, D_{23} is a continuous piecewise analytical combination of algebraic and inverse trigonometric functions^[8].

Substituting the matrix elements by the 2×2 matrices,

the secular equation with $n \times n$ complex matrix $H - ES$ (n is the number of electron bands in model of crystal under the consideration) is transformed into the secular equation with $2n \times 2n$ real matrix $\tilde{H} - E\tilde{S}$. As the Hamiltonian is a complex Hermitian negative definite matrix, whereas the overlap integrals matrix is a real symmetric positive definite, it is possible to rearrange the transformed secular equation in the standard form $\det(b - \epsilon\delta) = 0$. Here, the reduced Hamiltonian $b = \sigma^{-1} \tilde{H} \sigma^{-1}$ is a real symmetric positive defined matrix,

$$\sigma_{ii} = \sqrt{\tilde{S}_{ii} - \sum_{k=1}^{k=i-1} \sigma_{ik}^2} \quad i=1,2,3,\dots,2n$$

$$\sigma_{ij} = (\tilde{S}_{ij} - \sum_{k=1}^{k=j-1} \sigma_{ik} \sigma_{jk}) / \sigma_{jj} \quad j=1,2,3,\dots,i-1;$$

δ is the identity matrix; and ε is the absolute value of electron energy. This secular equation reduced to set of $(2n)^2$ quadric equations

$$\sum_{k=1}^{k=2n} (v_{ki} v_{kj} + \text{sgn}(i-j) v_{ik} v_{jk}) - b_{ij} = 0$$

$$i, j = 1, 2, 3, \dots, 2n$$

$$b_{ij} = \sum_{k=1}^{k=2n} I_{ki} I_{kj}$$

$$I_{ii} = \sqrt{h_{ii} - \sum_{k=1}^{k=i-1} I_{ik}^2} \quad i=1,2,3,\dots,2n$$

$$I_{ij} = (h_{ij} - \sum_{k=1}^{k=j-1} I_{ik} I_{jk}) / I_{jj} \quad j=1,2,3,\dots,i-1,$$

which in the initial quasi-classical approximation admits a solution by means of convergent iteration process^[9]. Using the obtained matrix elements v_{ij} the roots of the secular equation ε_i – electron states ionization potentials (for the fixed quasi-momentum vector) – are calculated as

$$\varepsilon_i = \sum_{k=1}^{k=2n} v_{ik}^2 \quad i=1,2,3,\dots,2n$$

In case of model inner potential (in form of analytical solution of Thomas–Fermi equation) the quasi-classically determined energetic parameters of system are shown to differ from their exact values by the multiplier of $(3\pi/10)^{2/3} \approx 0.96$. So, the expected errors of the quasi-classical approach make up a few

percent what is quite acceptable for the materials science purposes. And what is more, as the quasi-classical atomic radii are the finite parameters the quasi-classical matrix elements in secular equation for crystalline electronic structure contain a finite number of nonzero summands, which can be calculated analytically using the universal geometric functions. Thus, the quasi-classical approach is free from ambiguous errors arisen from series termination.

RESULTS

Applying the stated relations we have calculated the numerical values of Z_p , r'_i, r''_i , \tilde{r} , r_k and φ_k by fitting quasi-classical energy levels E_i to the Hartree–Fock ones^[10]. The requested quasi-classical parameters of the constituent atoms B and N are listed in TABLES 1 and 2.

The lattice constant value of $a=2.537 \text{ \AA}$ used in present calculation was previously found^[11] by minimization of the quasi-classically calculated w-BN crystal total energy fixing the ratio of lattice constants a and c , and internal parameter u at the ‘ideal values’: $(a/c)^2 = u = 3/8$. The accuracy of this lattice constant is remarkable: its deviation from the experimental one is only $\sim 0.6\%$. This fact allows us to conclude that quasi-classical method would be also preferable for estimations of energy differences characterizing wurtzite-like boron nitride electronic struc-

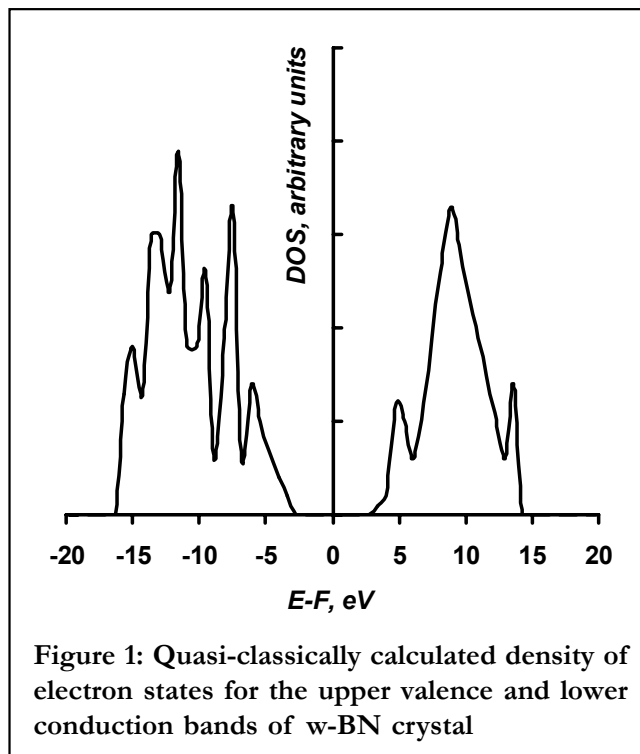
TABLE 1: Electrons and nucleus-electron cloud relative motion classical turning points radii in atoms B and N (in au)

| Atoms | B | | N | |
|--------------------------|-------------|------------------------|-------------|------------------------|
| | 0 or r'_i | \tilde{r} or r''_i | 0 or r'_i | \tilde{r} or r''_i |
| States | | | | |
| Nucleus – Electron Cloud | 0 | 0.027585 | 0 | 0.009446 |
| 1s | 0 | 0.509802 | 0 | 0.357724 |
| 2s | 0 | 4.021346 | 0 | 2.909074 |
| 2p | 0.744122 | 4.337060 | 0.549803 | 3.204489 |

TABLE 2: Quasi-classical parameters of the potential distributions in atoms B and N (in au)

| Atoms | B | | N | | |
|-------|---|----------|-------------|----------|-------------|
| | k | r_k | φ_k | r_k | φ_k |
| | 1 | 0.027585 | 210.5468 | 0.009446 | 878.4581 |
| | 2 | 0.509802 | 8.882329 | 0.357724 | 20.22523 |
| | 3 | 0.744122 | 3.652920 | 0.549803 | 8.464698 |
| | 4 | 4.021346 | 0.206072 | 2.909074 | 0.509668 |
| | 5 | 4.337060 | 0.000614 | 3.204489 | 0.003993 |

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ture.

The full basis set consisting of the occupied and empty valence orbitals of unit cell constituent atoms (B1, N1, B2, N2: $2s$, $2p$) is employed and the crystalline potential is represented by a sum of atom-centered step-like functions. On the ground of above described quasi-classical approach the solutions for the relevant secular equation have been obtained. Calculated DOS for w-BN upper valence and lower conduction bands with respect to Fermi level is shown in the figure 1. It reveals that w-BN is an insulator with band gap of $E_g = 5.4\text{eV}$.

DISCUSSION AND CONCLUSIONS

Boron and nitrogen atoms are tetrahedrally surrounded in both of densely packed forms of boron nitride and in 'ideal case', that mimics the real one, the w-BN structure differs from the c-BN structure only in the stacking sequence of the B and N atoms. Correspondingly, the nearest-neighbor atomic environments and bonding types in both crystals are sufficiently close and it has been taken for granted that their electronic structures are also similar. However, the lower symmetry and small deviations of bond lengths in the w-BN structure can result in some

TABLE 3: w-BN bandwidths theoretical values (in eV)

| Upper valence band | Band gap | Lower conduction band | Method | Reference |
|--------------------|----------|-----------------------|--------|-----------|
| 11.0 | 4.9 | $\sim 11.5^a$ | FLAPW | [20] |
| $\sim 11.5^a$ | 5.81 | $> 8.0^a$ | OLCAO | [21] |
| 11.76 | 5.81 | $\sim 11.0^a$ | OLCAO | [22] |
| — | 5.45 | — | LMTO | [23] |
| 13.6 | 5.4 | 11.6 | QC | this work |

^a estimations made from the given DOS-curves

unique features of its electronic properties. It urges on analysis of w-BN in comparison with c-BN.

Indeed there are found^[12,13] substantial differences in the B and N X-ray spectra of w-BN and h-BN, and to a lesser extent between w-BN and c-BN. According to these early experiments the band gap for wurtzite-type boron nitride equals to $E_g = 2.1\text{eV}$ which confirms that w-BN is an insulator^[14]. But, it seems that this value underestimates the real one indicating low-quality crystals. The valence electrons X-ray emission spectra obtained for h-BN, c-BN, w-BN crystals, and the product of plasma-chemical synthesis including all of boron nitride phases also reveal the similarity of w-BN and c-BN electronic structures^[15]. The electronic excitation spectra for the three boron nitride modifications under applied pressure and lattice stretching up to stresses $\sim 0.01\text{Mbar}$ show same fundamental gap ordering that found at equilibrium^[16]. Slight differences between the K-emission spectra of boron nitride denser modifications may be recognized by the analysis based on X_α -method^[17] or calculations within the local coherent potential approximation(LCPA)^[18,19]. The last allows obtaining the fine structure in the region of top of valence bands in the corresponding crystals and shows that fine structure for w-BN is in a less degree pronounced.

Park et al^[20] were the first to calculate electronic structure for w-BN. By means of full potential linear augmented plane wave (FLAPW) method they found that like the boron nitride another crystalline modifications w-BN is an insulator with the indirect gap produced by the valence band maximum at Γ point and the conduction band minimum at K point. Xu and Ching^[21,22] presented the DOS of w-BN in comparison with other boron nitrides and some

wurtzite-like crystals using orthogonalized linear combination of atomic orbitals (OLCAO) method in the local-density approximation (LDA). Linear muffin tin orbital (LMTO) band structure calculations were applied by Christensen and Gorczya^[23] to investigate optical properties of the boron nitride in the wurtzite structure under hydrostatic pressure. All of DOS-curves calculated for w-BN, including the quasi-classically (QC) found one, in outline are similar. But, main peaks positions agree only qualitatively. The w-BN electron bandwidths theoretical values are compiled in TABLE 3. They show the identical trend, with a narrow spread.

The obtained quasi-classical DOS-curve and its parameters (upper valence and lower conduction bandwidths, and gap between them) would be useful for investigations of wurtzite-like boron nitride electronic properties.

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